Charge Photogeneration and Recombination in Organic Semiconductors, Lewis Rothberg, University of Rochester, DMR0309444

Processible semiconducting organic materials are attractive candidates to make large area solar cells. The requirement for efficient charge photogeneration is that all absorption occur near (< 10 nm from) the interface between donor and acceptor molecular units so that the initially created excited state is separated into an electron and hole. At the same time, these charges must be extracted from the device without recombination. It would be optimal to organize the donors and acceptors to provide continuous paths for charges to escape the cell. We are synthesizing soluble fan-shaped tree-like molecules (dendrimers) with conducting oligomeric branches (Fig. 1 top) that will serve as donor and acceptors. The donors have thiophene branches (p-type) and the acceptors thiazole branches (n-type) and each will be around 10 nm in size. The two dendrimers will be chemically linked (Fig. 1 bottom) and their peripheries functionalized to encourage organized phase segregation into columns as illustrated schematically. The use of a dendritic architecture enables well defined dimensions and the ability to use the cores to define the electronic properties while the periphery regulates the solubility and solid state morphology.

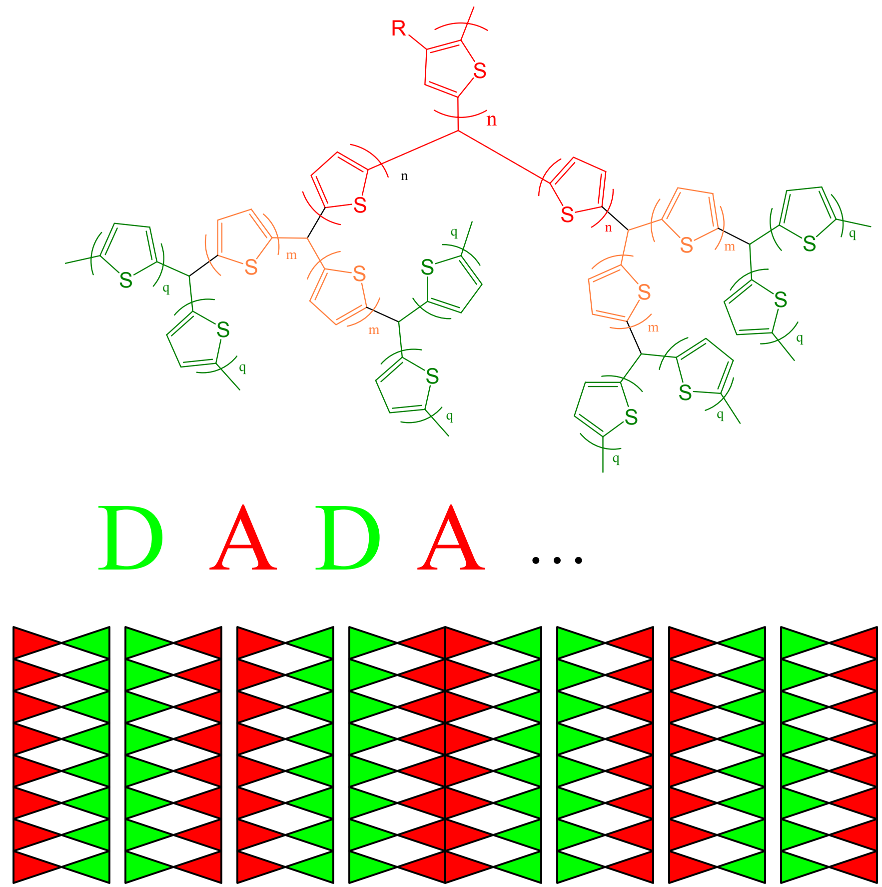

Fig. 1. Organized phase segregation to form bicontinuous donor and acceptor networks from p-type and n-type thiophene and thiazole dendrimers.

Renewable energy sources are extremely important and organic solar cells appear to be commercially promising because they can be processed into large area films. The relatively poor charge transport in organic materials, however, means that recombination of photogenerated charges simply resulting in heat makes for poor efficiency. Our strategy is to provide conductive paths to the electrodes so that electrons do not encounter photogenerated holes. The idea is to use organized phase segregation to make these paths. The dimensions of the paths, however, are dictated by the requirement that absorbed light must be close to an interface between the acceptor and donor molecules in order for the excited state to be split into charges. This dimension must be no more than about 10 nanometers. In the scheme we are working towards, both the individual donor acceptor pair spacing and the overall organization of donor acceptor pairs will be determined by the dendritic architecture. This is in contrast to doped polymer based solar cells that are currently the most efficient of the all organic solar cells where the dimensions are not well controlled. Yong Zhang (graduate student) has finished synthesizing the p-type dendrimer which is based on oligothiophene branches since these are good conductors and absorb throughout the visible region of the spectrum. He is doing the optical characterization and writing up this work while one of Prof. Ng's students has started on the n-type dendrimers. He has also set up a testbed to measure solar (photovoltaic) cell properties so that we are able to assess devices made from these materials and compare them to commercially available silicon devices.

The grant also supports Jane Wesely's work on oligofluorene photophysics (in particular, persistent photoluminescence) which is designed to understand how much charge is photogenerated and how much of the photoluminescence comes from recombination of photogenerated charges. This is an important issue for electroluminescent device materials because it means that measurements of photoluminescence quantum yield do not correctly estimate what the EL efficiency would be. It also sets up an ideal situation to study charge recombination in a situation where there are no contacts to complicate interpretation and one can work at low temperature where it is easy to see phosphorescence. Her recent results indicate that even in this nominally homogenous material, there is a large amount (> 10 %) of charge photogeneration and that many of these charges become triplet states that do not emit light.

Finally, we are also studying the properties of single polymer chains to understand how they fold back on themselves and how this depends on solvent. We have found that chains deposited onto a substrate "remember" their solution configuration so that the solvent from which they are cast has important effects on devices. This information comes from fluorescent and Raman studies of single chains of MEH-PPV by postdoctoral student Zhenjia Wang who is partially supported by the grant. In order to do this work, we have advanced the understanding of the nanotextured silver surfaces required to observe single molecule Raman scattering. This in turn has led to the ability to observe remarkable phenomena such as chemical bond breakage and formation in single molecules. Potential applications to development of highly sensitive molecularly specific sensors may be one long term result of the work.

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Education:

The highlighted work has been done by a graduate student Yong Zhang in collaboration with a synthetic chemist Prof. Man Kit Ng. The NSF grant also supports graduate student Jane Wesely and postdoctoral student Zhenjia Wang who work on photoinduced charge generation in conjugated oligofluorenes and poly paraphenylenevinylenes respectively. REU student Rosana Pompey and RET high school teachers Jude Ndambuke and Robert Meek have also participated in research related to this grant over the past two years. Rothberg's group has hosted fifteen RET, REU and CIRE participants over the last seven summers. Rothberg also belongs to the CCNY IGERT and has done coordinated televised seminars with the Center for Analysis of Structures and Interfaces at minority-serving institution CCNY. Five CIRE students from CCNY done summer research with the group. Rothberg leads a materials cluster consisting of five faculty groups within the Chemistry department to broaden student education and foster interdisciplinary interactions.

Outreach:

The PI participates in a wide variety of community activities including science Saturdays at the Rochester Science museum and judging at high school science fairs. Local high school students were hired for summer research in each of the last two years. One is presently using his work for the Westinghouse competition.

The PI is advisor to the undergraduate ACS council who put on a show for high schools in the community where over 100 students attend annually.